

Appendix A

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    <?xml version="1.0" encoding="UTF-8" ?>
  - <model name="FieldKorosNoyesModel">
  - <notes>
5 <h1>Field-Koros-Noyes Model of BZ Reaction</h1>
  - <table border="0" cellspacing="0" cellpadding="2">
  - <thead>
  - <tr>
    <th align="left" valign="middle" bgcolor="#eeeeee">Citation</th>
10  </tr>
    </thead>
  - <tbody>
  - <tr>
  - <td>
15  R.J.Field and R.M.Noyes,J.Chem.Phys.60,1877 (1974) ;
    R.J.Field,E.Koros,R.M.Noyes,JACS 94,8649 (1972);R.J.Field, R.M.Noyes,Nature
    237,390 (1972) This implementation is taken manufactured by J.D. Murray,
    "Mathematical Biology" (1989) page 181.
    <a href="" />
20  </td>
    </tr>
    </tbody>
    </table>
  - <table border="0" cellspacing="0" cellpadding="2">
25 <thead>
  - <tr>
    <th align="left" valign="middle" bgcolor="#eeeeee">Description</th>
    </tr>
    </thead>
30 <tbody>
  - <tr>
    <td>Field Noyes Version of Belousov- Zhabotinsky Reaction. BrO3 is held
      constant; HOBr is typically ignored, and can be replaced by an empty- set. The
      stoichiometry f is typically taken as 1/ 2 or 1 (denominator 1 or 2 in SBML)
35  .</td>
    </tr>
    </tbody>
    </table>
  - <table border="0" cellspacing="0" cellpadding="2">
40 <thead>
  - <tr>
    <th align="left" valign="middle" bgcolor="#eeeeee">Rate constant    </th>
    <th align="left" valign="middle" bgcolor="#eeeeee">Reaction</th>
    </tr>
45  </thead>
  - <tbody>
  - <tr>
    <td>k1 = 1.3</td>
    <td>Br + BrO3 -> HBrO2 + HOBr</td>
50  </tr>

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- <tr>
  <td>k2 = 2000000</td>
  <td>Br + HBrO2 -> HOBr^2</td>
</tr>
5 <tr>
  <td>k3 = 34</td>
  <td>BrO3 + HBrO2 -> Ce^2 + HBrO2^2</td>
</tr>
- <tr>
10 <td>k4 = 3000</td>
  <td>HBrO2^2 -> BrO3 + HOBr</td>
</tr>
- <tr>
  <td>k5 = 0.02</td>
15 <td>Ce -> Br^f</td>
</tr>
</tbody>
</table>
- <table border="0" cellspacing="0" cellpadding="2">
20 <thead>
  - <tr>
    <th align="left" valign="middle" bgcolor="#eeeeee">Variable</th>
    <th align="left" valign="middle" bgcolor="#eeeeee">IC </th>
    <th align="left" valign="middle" bgcolor="#eeeeee">ODE</th>
25 </tr>
  </thead>
  - <tbody>
  - <tr>
    <td>Br</td>
30 <td>0.003</td>
    <td>Br'[t] == -(k1*Br[t]*BrO3[t]) + f*k5*Ce[t] - k2*Br[t]*HBrO2[t]</td>
    </tr>
  - <tr>
    <td>Ce</td>
35 <td>0.05</td>
    <td>Ce'[t] == -(k5*Ce[t]) + 2*k3*BrO3[t]*HBrO2[t]</td>
    </tr>
  - <tr>
    <td>HBrO2</td>
40 <td>0.001</td>
    <td>HBrO2'[t] == k1*Br[t]*BrO3[t] - k2*Br[t]*HBrO2[t] +
      k3*BrO3[t]*HBrO2[t] - k4*HBrO2[t]^2</td>
    </tr>
  - <tr>
    <td>HOBr</td>
45 <td>0</td>
    <td>HOBr'[t] == k1*Br[t]*BrO3[t] + 2*k2*Br[t]*HBrO2[t]
      + k4*HBrO2[t]^2</td>
    </tr>
50 </tbody>
</table>
</body>

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10 <specie name="Ce" initialAmount="0.05" compartment="BZ" boundaryCondition="false"
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- <listOfProducts>
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- <reaction name="Reaction2" reversible="false">
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- <listOfProducts>
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40 </listOfProducts>
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45 </kineticLaw>
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- <reaction name="Reaction3" reversible="false">
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- <listOfProducts>

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  </reaction>
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  - <kineticLaw formula="Ce*k5">
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    <parameter name="k5" value="0.02" />
    <parameter name="f" value="0.5" />
35 </listOfParameters>
    </kineticLaw>
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40 </sbml>

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